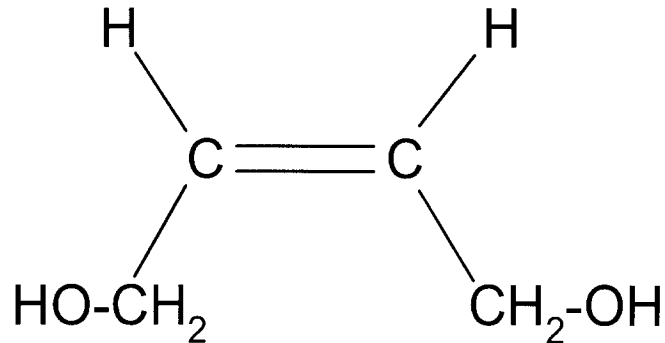


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2-Butene-1,4-diol

**CAS Number 110-64-5**

Existing Chemical	: ID: 110-64-5
CAS No.	: 110-64-5
EINECS Name	: but-2-ene-1,4-diol
EC No.	: 203-787-0
TSCA Name	: 2-Butene-1,4-diol
Molecular Formula	: C4H8O2

Producer related part	
Company	: Toxicology and Regulatory Affairs
Creation date	: 26.12.2002

Substance related part	
Company	: Toxicology and Regulatory Affairs
Creation date	: 26.12.2002

Status	:
Memo	:

Printing date	: 31.12.2002
Revision date	:
Date of last update	: 31.12.2002

Number of pages	: 28
-----------------	------

Chapter (profile)	: Chapter: 1.0.1, 1.2, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.3.2, 3.5, 4.1, 4.2, 4.3, 4.4, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.7, 5.8.1, 5.8.2
Reliability (profile)	: Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	: Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 110-64-5

Date 31.12.2002

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : lead organisation
Name : Toxicology and Regulatory Affairs
Contact person : Elmer Rauckman PhD DABT
Date :
Street : 1201 Anise Court
Town : Freeburg, IL
Country : United States
Phone : 618-539-5280
Telefax : 618-539-5394
Telex :
Cedex :
Email : rauckman@toxicsolutions.com
Homepage : toxicsolutions.com

Remark : Participating Members of Consortium

BASF Corporation
International Specialty Products

31.12.2002

1.2 SYNONYMS AND TRADENAMES

2. Physico-Chemical Data

Id 110-64-5

Date 31.12.2002

2.1 MELTING POINT

Value : = 10 °C
Sublimation :
Method :
Year :
GLP : no data
Test substance :

Test substance : 2-Butene-1,4-diol CASNO 110-64-5
Reliability : (2) valid with restrictions
Handbook values are assigned level 2
Flag : Critical study for SIDS endpoint
27.12.2002

(19)

2.2 BOILING POINT

Value : = 240 °C at 1013 hPa
Decomposition : yes
Method :
Year :
GLP :
Test substance :

Remark : Material deteriorates above 180 deg C.
Test substance : 2-Butene-1,4-diol CASNO 110-64-5
Reliability : (2) valid with restrictions
Handbook values are assigned level 2
Flag : Critical study for SIDS endpoint
27.12.2002

(19)

2.3 DENSITY

Type : relative density
Value : = 1.067 - 1.074 at °C

Test substance : 2-Butene-1,4-diol CASNO 110-64-5
Reliability : (2) valid with restrictions
Handbook values are assigned level 2
27.12.2002

(25)

2.4 VAPOUR PRESSURE

Value : = .0087 hPa at 25 °C

Remark : This is an experimental value

Value supported by MPBPWIN v1.40 estimates

2. Physico-Chemical Data

Id 110-64-5

Date 31.12.2002

Vapor Pressure Estimations (25 deg C):
(Using BP: 233.00 deg C (user entered))
(MP not used for liquids)
VP: 0.00661 mm Hg (Antoine Method)
VP: 0.00579 mm Hg (Modified Grain Method)
VP: 0.109 mm Hg (Mackay Method)
Selected VP: 0.0062 mm Hg (Mean of Antoine & Grain methods)

Test substance : 2-Butene-1,4-diol CASNO 110-64-5
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

27.12.2002

(16)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = -.9 at 25 °C
pH value :
Method : other (measured)
Year :
GLP : no data
Test substance :

Method : Three defined quantities of test material were weighed and dissolved in three aliquots of 25 ml 1-octanol. Each was allowed to equilibrate with 25 ml of distilled water at 25° C. The amount of test material in each phase was determined in triplicate using a gc method with an external standard.

Result : Results of the first trial triplicate determinations were

TS in octanol 0.744, 0.744, 0.735 average 0.741 g/L
TS in water 6.064, 6.029, 5.995 average 6.029 g/L
Po/w = 0.123

Results of the second trial triplicate determinations were

TS in octanol 1.132, 1.131, 1.334 average 1.132 g/L
TS in water nd 8.817, 8.842 average 8.830 g/L
Po/w = 0.128

Results of the third trial triplicate determinations were

TS in octanol 1.492, 1.496, 1.502 average 1.497 g/L
TS in water 11.608, 11.514, 11.363 average 11.495 g/L
Po/w = 0.130

Mean Po/w = 0.127

Log Po/w = -0.90

Test substance : 2-Butene-1,4-diol CASNO 110-64-5 Purity 99.3%
Reliability : (1) valid without restriction
Although the method differs in concentration range from the current OECD 107, it was conducted at three concentration levels and by a scientifically defensible method.

Flag : Critical study for SIDS endpoint

29.12.2002

(14)

2. Physico-Chemical Data

Id 110-64-5

Date 31.12.2002

Partition coefficient : octanol-water
Log pow : -.81 at °C
pH value :

Remark : Supporting Data
Test substance : 2-Butene-1,4-diol CASNO 110-64-5
29.12.2002

(20)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : miscible
Stable :

Test substance : 2-Butene-1,4-diol CASNO 110-64-5
Reliability : (2) valid with restrictions
Handbook values are assigned level 2
Flag : Critical study for SIDS endpoint
30.12.2002

(26)

Solubility in : Water
Value : at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : very soluble (> 10000 mg/L)
Stable :

Test substance : 2-Butene-1,4-diol CASNO 110-64-5
Reliability : (2) valid with restrictions
Handbook values are assigned level 2
Flag : Critical study for SIDS endpoint
30.12.2002

(18)

3. Environmental Fate and Pathways

Id 110-64-5

Date 31.12.2002

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight

INDIRECT PHOTOLYSIS

Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .0000000000632 cm³/(molecule*sec)
Degradation : ca. 50 % after 2 hour(s)
Deg. product :
Method : other (calculated)
Year : 2002
GLP : no
Test substance :

Method : Calculated using AOP version 1.90. Based on 12-hour day and EPA default of 1.5E6 OH/cm³.

Remark : Commercial material is mainly cis isomer

Result

AOP Program (v1.90) Results:

=====

SMILES : OCC=CCO

CHEM : Butenediol

MOL FOR: C4 H8 O2

MOL WT : 88.11

----- SUMMARY (AOP v1.90): HYDROXYL RADICALS -----

Hydrogen Abstraction = 6.5380 E-12 cm³/molecule-sec

Reaction with N, S and -OH = 0.2800 E-12 cm³/molecule-sec

Addition to Triple Bonds = 0.0000 E-12 cm³/molecule-sec

Addition to Olefinic Bonds = 56.4000 E-12 cm³/molecule-sec [Cis-isomer]

Addition to Olefinic Bonds = 64.0000 E-12 cm³/molecule-sec [Trans-isomer]

Addition to Aromatic Rings = 0.0000 E-12 cm³/molecule-sec

Addition to Fused Rings = 0.0000 E-12 cm³/molecule-sec

OVERALL OH Rate Constant = 63.2180 E-12 cm³/molecule-sec [Cis-isomer]

OVERALL OH Rate Constant = 70.8180 E-12 cm³/molecule-sec [Trans-isomer]

HALF-LIFE = 2.030 Hrs (12-hr day; 1.5E6 OH/cm³) [Cis-isomer]

HALF-LIFE = 1.812 Hrs (12-hr day; 1.5E6 OH/cm³) [Trans-isomer]

As the commercial material is predominantly the cis isomer, the cis data are given as the result

Source : Calculation by Toxicology and Regulatory Affairs, December 2002

Test substance : 2-Butene-1,4-diol CASNO 110-64-5

Reliability : (2) valid with restrictions
Calculated by an acceptable method

Flag : Critical study for SIDS endpoint

30.12.2002

(2)

3. Environmental Fate and Pathways

Id 110-64-5

Date 31.12.2002

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : O3
Conc. of sensitizer : 700000000000 molecule/cm³
Rate constant : ca. .00000000000000013 cm³/(molecule*sec)
Degradation : ca. 50 % after 2.1 hour(s)

Method : Calculated using AOP version 1.90. Based on 12-hour day and default ozone concentration of at 7E11 ozone mol/cm³.
Remark : Commercial material is mainly cis isomer
Result :
AOP Program (v1.90) Results:
=====
SMILES : OCC=CCO
CHEM : Butenediol
MOL FOR: C4 H8 O2
MOL WT : 88.11

----- SUMMARY (AOP v1.90): OZONE REACTION -----
OVERALL OZONE Rate Constant = 13.000000 E-17 cm³/molecule-sec
[Cis]
OVERALL OZONE Rate Constant = 20.000000 E-17 cm³/molecule-sec
[Trans]

HALF-LIFE = 2.116 Hrs (at 7E11 mol/cm³) [Cis-isomer]*
HALF-LIFE = 1.375 Hrs (at 7E11 mol/cm³) [Trans-isomer]

*As the commercial material is predominantly the cis isomer, the cis data are given as the result
Source : Calculation by Toxicology and Regulatory Affairs, December 2002
Test substance : 2-Butene-1,4-diol CASNO 110-64-5
Reliability : (2) valid with restrictions
Calculated by an acceptable method
Flag : Critical study for SIDS endpoint
30.12.2002 (2)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Degradation : < 50 % after 1 year at pH and °C

Method : The stability of this material in water is estimated based on established chemical principles.
Result :
Both the alkene and alcohol moieties are considered resistant to hydrolysis by Harris (J.C. Harris in Lyman W, Reehl, W and Rosenblat, D. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington D.C. 1990, page 7-6). This indicates a hydrolytic half-life of greater than one year.

3. Environmental Fate and Pathways

Id 110-64-5

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To verify this determination any possible interactions between individual chemical moieties are also considered. Although some alkenes are known undergo acid catalyzed hydration, these generally have structures that allow the formation of the more energetically favorable tertiary carbocation. In the case of 2-butene-1,4-diol, the carbocation would be the less favorable secondary ion. Furthermore, the alcohol free electron pairs would buffer the system to acid catalysis of the power necessary to form the secondary carbocation. The position of the hydroxyls is also unfavorable to add resonance stabilization to a secondary carbocation (see Vollhardt, K. "Organic Chemistry" WH Freeman and Co, New York, 1987). Thus, even though the hydration reaction of olefins with water is known in the chemical literature, the reaction is highly unfavorable for this material.

In summary, 2-Butene-1,4-diol is considered resistant to hydrolysis and will have an environmental hydrolytic half-life greater than one year.

Source : Estimated by Toxicology and Regulatory Affairs chemist based on acceptable chemical principles
Test substance : 2-Butene-1,4-diol CASNO 110-64-5, Cis 97.5%, Trans 2.0%
Reliability : (2) valid with restrictions
Calculated by an acceptable method
Flag : Critical study for SIDS endpoint

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(21)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year : 2002
Method : EQC Level 3 calculation using EPIWIN 3.05 with measured values of physical parameters and biodegradation times validated by data. Air lifetime adjusted for reaction with hydroxyl radical and ozone. See results for values employed

Result : Level III Fugacity Model (Full-Output):
=====

Chem Name : Butenediol
Molecular Wt: 88.11
Henry's LC : 2.03e-007 atm-m3/mole (Henrywin program)
Vapor Press : 0.0062 mm Hg (Mpbpwin program)
Log Kow : -0.9 (user-entered)
Soil Koc : 0.0516 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.38	1.39	1000
Water	53.5	208	1000
Soil	46	208	1000
Sediment	0.080	832	0

3. Environmental Fate and Pathways

Id 110-64-5

Date 31.12.2002

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	5.49e-012	986	19.8	32.9	0.66
Water	3.19e-012	923	277	30.8	9.24
Soil	1.01e-010	793	0	26.4	0
Sed't	2.38e-012	0.344	0.008	0.012	0.0003

Persistence Time: 173 hr
Reaction Time: 192 hr
Advection Time: 1.74e+003 hr
Percent Reacted: 90.1
Percent Adverted: 9.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 1.391
Water: 208.1
Soil: 208.1
Sediment: 832.3
Biowin estimate: 3.324 (days-weeks)

Advection Times (hr):

Air: 100
Water: 1000
Sediment: 5e+004

Source : Calculation by Toxicology and Regulatory Affairs
Test substance : 2-Butene-1,4-diol CASNO 110-64-5, Cis 97.5%, Trans 2.0%
Reliability : (2) valid with restrictions
Calculated by an acceptable method
Flag : Critical study for SIDS endpoint
30.12.2002

(17)

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, industrial
Concentration : 196.6 mg/l related to DOC (Dissolved Organic Carbon)
related to
Contact time : 8 day(s)
Degradation : ca. 99 (±) % after 3 day(s)
Result :
Deg. product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens
Test"
Year :
GLP : no data
Test substance :

Method : The study was conducted according to OECD Guideline 302 B using
activated sludge from a BASF water treatment plant. The initial value for
the test substance DOC was 196.6 mg/L. DOC was determined in test and
blank cultures daily for 8 days.

Result : Elimination of organic carbon from the test material was rapid. The percent
elimination on days 1-8 were 15%, 95%, 99%, 97%, 98%, 99%, 97% and
98% when calculated by taking the difference between the test and blank
culture DOC levels after centrifugation.

3. Environmental Fate and Pathways

Id 110-64-5

Date 31.12.2002

Test substance : 2-Butene-1,4-diol CASNO 110-64-5

Conclusion :
Inherently biodegradable

Reliability : (1) valid without restriction
Guideline study with no deviations.

Flag : Critical study for SIDS endpoint

30.12.2002

(1)

Type : aerobic

Inoculum :

Contact time : 30 day(s)

Degradation : = 67 (±) % after 30 day(s)

Result :

Kinetic of testsubst. : 5 day(s) = 2.7 %
15 day(s) = 9.3 %
30 day(s) = 67 %
%
%

Method : A closed bottle test was used and it was described as a "GF Test" Oxygen consumption was monitored at 5, 15 and 30 days.

Remark : Details of the testing procedure were not provided

Test substance : 2-Butene-1,4-diol CASNO 110-64-5

Conclusion :

In the report it was stated that based on the 67% degradation, it can be concluded that this material is completely degradable in a normally operating clarification plant.

Reliability : (4) not assignable

30.12.2002

(22)

4. Ecotoxicity

Id 110-64-5

Date 31.12.2002

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Leuciscus idus (Fish, fresh water)
Exposure period :
Unit : mg/l
LC0 : = 300
LC50 : = 390
LC100 : = 500
Method : other: German Standard Method DIN 38412 L15
Year :
GLP : no
Test substance :

Method : Study followed method specified in German Standard Method DIN 38412 L15.

Test substance : 2-Butene-1,4-diol CASNO 110-64-5

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

30.12.2002

(22)

Type : static
Species : other: Lepomonis macrochirus, Carassius auratus, Salmo trutta
Exposure period : 4 hour(s)
Unit : mg/l

Method :
This study was designed to determine the "excess toxicity" of several alcohols over the toxicity predicted based on a simple narcosis mechanism of action. Alcohols (non phenolic) without heteroatoms were selected from previous aquatic toxicity screening studies and were compared to their predicted toxicity using the Könemann QSAR relationship (Könemann, H. Toxicology 19:223-228,1981) for death by narcosis.

Remark :
Actual conclusions about the toxicity of butanediol are impossible to draw from this publication as there are several important deficiencies including, the predicted toxicity of the test substance was not given; the predicted toxicity is based on the log Ko/w, which is erroneously given in the paper as -1.67. Use of this incorrect log Ko/w would make butenediol appear even less toxic using the Könemann equation. Using the ECOSAR neutral organics model with a log ko/w of -0.90, produces a predicted fish 96-hour LC50 of 32,500 mg/L.

Due to these issues, no conclusions can be drawn about the toxicity of the test material from this study.

Result :
The investigators found data for butenediol on three species of fish Lepomonis macrochirus, Carassius auratus, and Salmo trutta. These data were from a screening study at a single concentration of 5 mg/l (data from Hollis/Wood US Fish and Wildlife Service reports on toxicity of chemicals to fish). The data indicate that at 5 mg/L, all three species displayed signs of "sickness" but not death. The "sickness" was reported at 4 hours of treatment, it couldn't be determined if observation were made out to 24 hours or if the study was terminated after 4 hours.

Conclusion :

4. Ecotoxicity

Id 110-64-5

Date 31.12.2002

From the data indicating effects at 5 mg/kg, the authors concluded that butenediol produces "excess" toxicity.

Reliability : (4) not assignable (27)
28.12.2002

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC0 : = 31.3
EC50 : = 65.2
EC100 : = 125
Limit Test : no
Analytical monitoring : no
Method : Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year :
GLP : no data
Test substance :

Method : Groups of 20 daphnids (4 replicates of 5 animals) were exposed to eight nominal concentrations of test substance for a period of 48 hours. Animals (2 to 24 hours old) were examined for immobilization at 0, 3, 6, 24, and 48 hours after starting the exposure.

Remark : Two issues are potential confounders in this study. The first is volatility; however, based on the vapor pressure and water solubility (Henry's Law Constant) of the test material, this is considered to not be an issue.

The second issue is water stability of the test material. As this material has no groups susceptible to hydrolysis, water stability is not considered to be an issue in this test.

Result : Animals were found to be immobilized at test concentrations of 62.5 mg/L and above. Initial pH was 7.97-8.25, final pH was 7.89 to 8.13 with lower values at higher concentrations of test substance. Temperature was 293.7° K. TOC was not reported. Oxygen concentration was measured in a parallel set of vessels and was above 7.4 mg/L in all concentrations at the beginning and end of the study.

Results are given as the number of swimming daphnia at 24 and 48 hours. Observations were also reported for 3 and 6 hours but there was no immobilization at these times.

Conc	24 hr	48 hr
0	20	20
3.8	20	20
7.8	20	20
15.6	20	20
31.3	20	20
62.5	20	11
125	18	0
250	4	0
500	0	0

4. Ecotoxicity

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Date 31.12.2002

Test condition : Vessels were glass centrifuge tubes containing 10 ml of test solution. The dilution water was filtered tap-water with the chlorine removed by passing the water over activated carbon and had a hardness of 2.7 mmol/L, an alkalinity of 0.80 mmol/L and Ratios of Ca: Mg of 4:1 and Na:K of 10:1. Lighting was diffuse 630 microSiemens/cm on a 16-hour light, 8-hour dark cycle. Initial pH of the dilution water was 7.9. The alkalinity and hardness of the tap water had be reduced with distilled water and sulfuric acid to attain the desired values.

Test substance : 2-Butene-1,4-diol CASNO 110-64-5 Purity > 98.5%

Reliability : (2) valid with restrictions
Guideline study without analytical measurements

Flag : Critical study for SIDS endpoint

30.12.2002 (11)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : *Scenedesmus subspicatus* (Algae)

Endpoint :

Exposure period : 72 hour(s)

Unit : mg/l

EC10 : = 48

EC50 : = 290

EC90 : = 1550

Limit test :

Analytical monitoring : no

Method : other: *Scenedesmus*-Zellvermehrungs-Hemmtest, DIN 38412 Teil 9, Bestimmung der Hemmwirkung von Wasserinhaltsstoffen auf Gruenalgen

Year :

GLP : no data

Test substance :

Method : Three days before the start of the test, algae cells were inoculated into fresh media (DIN 38 412 part 9) and allowed to reach exponential growth phase before inoculating the test flasks. The test flasks were inoculated with 10000 cells per ml. The stock solutions of test material were prepared in distilled water at 12 g/L or 1.2 g/L and diluted with growth media to give the following concentrations of test substance for the growth inhibition assay: 0, 0.6, 6.0, 60.0, 600, 6000 mg/L. Containers were test tubes containing 10 ml of test solutions. Four replicates of each dilution and eight replicates of the control solution were used. Algae were kept suspended by twice daily agitation with a test-tube shaker. Algal biomass was determined fluorometrically at initiation and after 24, 48 and 72 hours of incubation. Temperature of incubation was 20 deg C plus or minus one degree. Lighting was continuous at a level of ca 120 microE.

Result : The fluorometric measurements were averaged for each time and concentration and compared with control to determine the growth inhibition. Readings between replicates showed little variation and no deviations from the protocol were noted.

The following relative biomass quantities and percent inhibition of biomass were recorded

4. Ecotoxicity

Id 110-64-5

Date 31.12.2002

Conc	Biomass	% Inhibition
0	2.82	0
0.6 mg/L	3.08	-9.35
6.0	2.74	2.88
60	2.37	15.9
600	1.05	62.8
6000	0.00	100

The following derived parameters were determined graphically.

EC10 48 mg/L
EC50 290 mg/L
EC90 1550 mg/L

Test substance : 2-Butene-1,4-diol CASNO 110-64-5
Reliability : (2) valid with restrictions
Guideline study without analytical measurements
Flag : Critical study for SIDS endpoint

30.12.2002

(9)

Species : Scenedesmus subspicatus (Algae)
Endpoint :
Exposure period :
Unit : mg/l

28.12.2002

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type :
Species : activated sludge
Exposure period :
Unit :

Remark :
It was concluded that appropriate introduction into adapted biological purification plants will not disturb the activity of the activated sludge.

30.12.2002

(12)

Type :
Species : Pseudomonas putida (Bacteria)
Exposure period : 17 hour(s)
Unit : mg/l
EC10 : = 8934
EC50 : > 10000
EC90 : > 10000
Method : DIN 38412, part8
Year :
GLP :
Test substance :

30.12.2002

(10)

5. Toxicity

Id 110-64-5
Date 31.12.2002

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : = .8 ml/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle : water
Doses :
Method : other: BASF Method
Year :
GLP : no
Test substance :

Method : Animals were dosed by gavage and observed for 7 days
Remark : This calculates to be 856 mg/kg-bw as the LD50
Result :

At necropsy, it was reported that there was "suspicion of kidney toxicity".

Test substance : 2-Butene-1,4-diol CASNO 110-64-5
Reliability : (2) valid with restrictions
Conducted by a scientifically defensible method.

Flag : Critical study for SIDS endpoint

30.12.2002

(15)

Type : LD50
Value : = .45 ml/kg bw
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle : water
Doses :
Method : other: BASF Test
Year :
GLP :
Test substance :

Method : Animals were dosed by gavage and observed for 7 days

Remark : This calculates to an LD50 of 482 mg/Kg-bw

Test substance : 2-Butene-1,4-diol CASNO 110-64-5

30.12.2002

(15)

Type : other: Approximate ALD
Value :
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: BASF-Test
Year :
GLP : no
Test substance :

5. Toxicity

Id 110-64-5

Date 31.12.2002

Result	:	214 mg/kg was lethal to 0/2 535 mg/kg was lethal to 2/2	
Test substance	:	2-Butene-1,4-diol CASNO 110-64-5	
28.12.2002			(8)
Type	:	other: Approximate ALD	
Value	:		
Species	:	cat	
Strain	:		
Sex	:		
Number of animals	:		
Vehicle	:		
Doses	:		
Method	:	other: BASF-Test	
Year	:	1960	
GLP	:	no	
Test substance	:		
Remark	:	107 mg/kg letal bei 0/2; 214 mg/kg letal bei 2/2	
Result	:	at 107 mg/kg 0/2 animals died at 214 mg/kg 2/2 animals died	
28.12.2002			(8)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	other: Inhalation risk test	
Value	:	> 7 ppm	
Species	:	rat	
Strain	:		
Sex	:		
Number of animals	:		
Vehicle	:		
Doses	:		
Exposure time	:		
Method	:	Six rats were exposed to a saturated atmosphere of test material at 20 deg C, for a total of 8 hours. Mortality was recoded after 2 and 8 hours of exposure. Animals were observed for 8 days (including the day of exposure).	
Remark	:	Based on the established vapor pressure of 0.0089 hPa at 25° C, saturated air at 20° C would contain about 7 ppm test material.	
Result	:	No animal died during the exposure period or during the remainder of the 8-day exposure period. No adverse clinical signs were observed during exposure or after exposure.	
Test substance	:	2-Butene-1,4-diol CASNO 110-64-5	
Reliability	:	(2) valid with restrictions Conducted by a scientifically defensible method.	
28.12.2002			(13)

5. Toxicity

Id 110-64-5

Date 31.12.2002

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : > 200 mg/kg bw
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : other: DOT Guideline
Year :
GLP : no
Test substance :

Method :
Groups of 5 rabbits of each sex (males 2.95 kg, females 3.45 kg mean weight) received a single dose of 200 mg/kg-body weight test substance, without vehicle, to an area of about 50 sq cm. The areas was covered with an impermeable cover and the animals were wrapped with tape for a period of 15 to 24 hours at which time the tape and excess test substance was removed. Animals were observed for seven additional days. Animals were necropsied at the end of the observation period after sacrifice using carbon dioxide

Result :
No animal died during the exposure or the observation time. No adverse clinical signs were noted and no organ effects were found at necropsy.

Test substance : 2-Butene-1,4-diol CASNO 110-64-5
Reliability : (1) valid without restriction
Conducted by a scientifically defensible method.

30.12.2002 (5)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type : LD50
Value : = 327 mg/kg bw
Species : rat
Strain : Wistar
Sex : male/female
Number of animals : 30
Vehicle : physiol. saline
Doses : 3200, 3520, 3870, 4260, or 4680 micromoles/kg
Route of admin. : i.p.
Exposure time :
Method :
Year :
GLP : no
Test substance :

Method :
Groups of 6 adult Wistar albino rats (mixed sex) weighing 320-360 g were treated with the test substance in saline in i.p. injection at the following doses: 3200, 3520, 3870, 4260, or 4680 micromol/kg. Animals were observed for 18 hours to record mortality and body temperature and then for 24 hours longer. Rats were not necropsied.

5. Toxicity

Id 110-64-5

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Result : Results were as follows, doses given in micromoles per kg and have been converted to mg/kg for this summary.

D O S E

mcmol/kg	mg/kg	dead/total
3200	282	0/6
3520	310	1/6
3870	341	5/6
4260	375	5/6
4680	412	6/6

The 3200-mmol/kg dose induced few behavioral changes. Higher doses produced sedation and a loss of spontaneous activity 30-40 min. post-injection. These effects lasted 2-3 h, at which time most rats entered into tonic convulsions and died within 40 min. In rats that became sedated, there was no significant decrease in body temperature

Test substance : 2-Butene-1,4-diol CASNO 110-64-5

Reliability : (2) valid with restrictions

Acceptable publication

29.12.2002

(32)

Type : LD50

Value : = 480 mg/kg bw

Species : mouse

Strain :

Sex :

Number of animals :

Vehicle :

Doses :

Route of admin. : i.p.

Exposure time :

Method : other: BASF-Test

Year :

GLP : no

Test substance :

Test substance : 2-Butene-1,4-diol CASNO 110-64-5, Cis 97.5%, Trans 2.0%

29.12.2002

(7)

5.4 REPEATED DOSE TOXICITY

Type : Sub-acute

Species : rat

Sex : female

Strain : other: Albino

Route of admin. : oral feed

Exposure period : 13-days

Frequency of treatm. : continuous

Post exposure period : none

Doses : 5, 10, 20, 30, and 40 % as caloric value of diet

Control group : yes, concurrent no treatment

Method :

Year :

GLP : no

Test substance :

5. Toxicity

Id 110-64-5

Date 31.12.2002

Method	: This study was part of an investigation on the application of diols as synthetic nutrients. Diets were prepared with butenediol composing 5, 10, 20, 30, or 40 % of the diet on a caloric basis (based on 6.54 kcal/gram butenediol). This diet (and similar diets for six other diols) was fed to groups of 2 female rats at each dietary level for up to 8 weeks.												
Result	: Feeding butenediol to rats at these levels produced 100% mortality. The animals died on the following days. <table><tr><td>% in diet</td><td>survival time</td></tr><tr><td>5</td><td>7 and 10 days</td></tr><tr><td>10</td><td>7 and 13 days</td></tr><tr><td>20</td><td>6 and 7 days</td></tr><tr><td>30</td><td>2 days</td></tr><tr><td>40</td><td>2 days</td></tr></table> No rat fed diet containing butenediol lived more than 13 days. No information concerning body weights or organ effects is available.	% in diet	survival time	5	7 and 10 days	10	7 and 13 days	20	6 and 7 days	30	2 days	40	2 days
% in diet	survival time												
5	7 and 10 days												
10	7 and 13 days												
20	6 and 7 days												
30	2 days												
40	2 days												
Test substance 30.12.2002	: 2-Butene-1,4-diol CASNO 110-64-5 (29)												
Type	: Sub-acute												
Species	: rabbit												
Sex	: male/female												
Strain	: no data												
Route of admin.	: gavage												
Exposure period	: 3 Weeks												
Frequency of treatm.	: 5 days per week (max. of 14 treatments)												
Post exposure period	:												
Doses	: 107 and 214 mg/kg												
Control group	: no												
Method	: other												
Year	:												
GLP	: no												
Test substance	:												
Method	: The test material was administered to groups of 2 (?) rabbits by gavage at either 107 or 214 mg/kg-bw, 5 days/week for three weeks (the maximum was 14 treatments). Animals were observed for adverse clinical signs and hematology and liver-function tests were performed on surviving animals.												
Result	: The 214-mg/kg dose led to the death of the treated rabbits after 4 or 9 treatments. Clinical signs were restricted to hyperactivity and diarrhea. Animals in the 107-mg/kg group showed a reduction in erythrocyte count and hematocrit. Bromosulfophthalein liver function tests did not show any adverse effect of the test substance on liver function.												
Test substance Reliability 30.12.2002	: 2-Butene-1,4-diol CASNO 110-64-5 : (2) valid with restrictions Conducted by a scientifically defensible method. (8)												
Type	: Sub-chronic												
Species	: other: Rats, Hamsters, Monkeys												
Sex	:												

5. Toxicity

Id 110-64-5

Date 31.12.2002

Strain	:	
Route of admin.	:	inhalation
Exposure period	:	6 months
Frequency of treatm.	:	5 days a week
Post exposure period	:	
Doses	:	1, 3 or 10 mg per cubic meter
Control group	:	
Method	:	The effects of chronic exposure to atmospheres containing maleic-anhydride were assessed in Engle-hamsters, CD-rats, and Rhesus-monkeys with regard to the adequacy of the threshold limit value of 1mg/m ³ . The animals were exposed to the anhydride at either 1, 3, or 10mg/m ³ , 6 hours per day, 5 days per week, for a 6 month period.
Remark	:	This study is on the probable main metabolite of 2-Butene-1,4-diol and is supporting.
Result	:	The mortality rate was less than 10 percent in all treatment groups for all three species. Transient weight reductions were observed for the medium and high level doses. Dose related nasal and ocular irritations were observed in all three species, but no ophthalmologic changes were indicated. Nasal and pulmonary histology revealed reversible hyperplastic, metaplastic, and inflammatory changes. Maleic-anhydride exposure had no significant effect on hemoglobin, hematocrit, total erythrocyte count, total and differential leukocyte counts, glucose, urea nitrogen, serum glutamic-pyruvic-transaminase activity, serum alkaline-phosphatase activity, carbon-dioxide, or erythrocyte, plasma, and terminal brain cholinesterase activities. Urine volume, pH, specific gravity, albumin, glucose, bilirubin, ketones, occult blood, and sediment were comparable in the exposed and control groups. No significant effects attributable to maleic-anhydride were determined from pulmonary function tests
Test substance	:	Maleic Anhydride CASNO 108-31-6
Reliability	:	(2) valid with restrictions
30.12.2002		(30)
Type	:	Chronic
Species	:	
Sex	:	
Strain	:	
Route of admin.	:	oral feed
Exposure period	:	2 years
Frequency of treatm.	:	continual
Post exposure period	:	
Doses	:	10, 32 and 100 mg/kg/day
Control group	:	yes, concurrent vehicle
Method	:	Rats (504 males, 501 females) were exposed to maleic anhydride in the diet at 0, 10, 32 and 100 mg/kg/day for two years.
Remark	:	This study is on the probable main metabolite of 2-Butene-1,4-diol and is supporting.
Result	:	Significant differences between treated and control animals were observed in the following: red blood cell count (at 6 months, decreased in males at all dose levels, females at high and low dose levels; at 12 months, decreased for males at low dose), hematocrit levels (at 6 months, decreased for males at high and low doses). Thyroid clear cell adenomas and hyperplasia were observed in females at all doses but it was not considered treatment

5. Toxicity

Id 110-64-5

Date 31.12.2002

related. There were no significant differences between treated and control animals in the following: body and organ weights, mortality, neurology, ophthalmology, or urinalysis. A NOEL was not established.

Test substance : Maleic Anhydride CASNO 108-31-6 (23)
30.12.2002

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium; TA98 TA100 TA1535 TA1537
Test concentration : 20 - 5000 ug/plate
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 1983
GLP : no
Test substance :

Method : S. typhimurium strains TA1535, TA100, TA1537, TA98 were tested using a plate incorporation technique and a preincubation technique both with and without metabolic activation. Aroclor 1254 induced rat liver S-9 was used for metabolic activation at a rate of 0.5 ml S-9 mix per plate when used with the overlay procedure or the preincubation procedure. In the plate-incorporation tests, test and control materials were incorporated directly into the overlay agar with the bacteria. In the preincubation assay, 0.5 ml S-9 mix, 0.1 ml bacteria suspension and 0.1 ml test or control material are mixed and incubated for 20 minutes before 2 ml of soft agar is added and the mixture poured on the agar plate.

Plates were prepared in triplicate using both the plate incorporation technique and the preincubation technique. After incubation at 37 ° C for 48 hours in the dark, colonies were counted.

Cytotoxicity of the test material to the bacteria was evaluated by the background lawn of bacteria and, in the presence of S-9, by determination of the "titer". For this, bacteria were diluted 10E-6 and mixed with S-9 and the two highest concentrations of the test material and plated on a maximal agar (with histidine) plate, incubated at 37° C for 48 hours and counted.

Concentrations tested were 0, 20, 100, 500, 2500 and 5000 micrograms per plate for all strains in both plate incorporation and preincubation assays. Test material was dissolved in distilled water and diluted to provide the correct level per plate.

The solvent and negative control substance was distilled water. Positive controls were:

Without metabolic activation:

MNNG (in DMSO) at 5 mcg/ plate for strain TA-1535 and TA-100

9-Aminoacridine at 100 mcg/ plate for strain TA-1537

4-Nitro-o-phenylenediamine 10 mcg/ plate for strain TA-98

With metabolic activation:

2-Aminoanthracene at 10 mcg/ plate for all strains

5. Toxicity

Id 110-64-5

Date 31.12.2002

	Statistical Methods
	Formal statistical methods were not used to evaluate the data. The following requirement generally need to be met for a substance to be characterized as positive:
	Doubling of the spontaneous mutation rate.
	Dose-response relationship
	Reproducibility of the results
Remark	: Year conducted: 1989
Result	: Slight cytotoxicity (less than 50%) was observed at the 5000 mcg/plate concentration for some strains in the presence of S9 using the "titer" method but no reduction in background bacterial lawns was observed on the test plates. The results of the plate incorporation and preincubation assays conducted on the test material at dose levels ranging from 20 to 5000 microliters per plate in the absence and presence of metabolic activation did not exhibit increased numbers of his+ revertant colonies. The positive control treatments in both the nonactivation and S9 activation assays for both the plate incorporation and preincubation techniques induced large increases in the revertant numbers with all the indicator strains, demonstrating the effectiveness of the S9 activation system and the ability of the test system to detect known mutagens.
Test substance	: 2-Butene-1,4-diol CASNO 110-64-5
Conclusion	: The test material, 2-Butene-1,4-diol, did not exhibit genetic activity in any of the assays conducted in this evaluation and was not mutagenic to the Salmonella typhimurium indicator organisms under the test conditions according to the established evaluation criteria.
Reliability	: (1) valid without restriction Guideline study under GLP with no deviations.
Flag	: Critical study for SIDS endpoint
30.12.2002	(6)
Type	: Ames test
System of testing	: Salmonella typhimurium TA 100; 98
Test concentration	: 20 - 5000 ug/plate
Cycotoxic concentr.	:
Metabolic activation	: with and without
Result	: negative
Method	: other: in Anlehnung an OECD Guide-line 471
Year	: 1983
GLP	: no
Test substance	:
Method	: The "liquid-suspension assay" was conducted as is sometimes shows enhanced sensitivity toward some mutagens that negative in the standard tests. In this test, 0.1 ml test solution or solvent, 1.5 ml bacterial suspension and 0.5 ml S-9 mix (or buffer) are incubated in tightly closed tubes in the shaking water bath at 37°C for about 90 minutes. Subsequently, the bacterial cultures are centrifuged at 5000 rpm for about 10 minutes, the supernatant is removed and 0.5 ml phosphate buffer (pH 7.4; 100 mM incl.

5. Toxicity

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150 mM KC1) and 2 ml of soft agar is added. After mixing and resuspending, the samples are poured onto Vogel-Bonner agar plates (minimal glucose agar plates, incubated at 37 ° C for 48 hours in the dark, and colonies counted. Incubations and plates were prepared and counted in triplicate. *S. typhimurium* strains TA100 and TA98 were tested using this procedure both with and without metabolic activation. Aroclor 1254 induced rat liver S-9 was used for metabolic activation.

Cytotoxicity of the test material to the bacteria was evaluation of the background lawn of bacteria.

Concentrations tested were 0, 20, 100, 500, 2500 and 5000 micrograms per plate for both strains. Test material was dissolved in distilled water and diluted to provide the correct level per tube.

The solvent and negative control substance was distilled water.

Positive controls were:

Without metabolic activation:

MNNG (in DMSO) at 5 mcg for strain TA-100

4-Nitro-o-phenylenediamine 10 mcg/ plate for strain TA-98

With metabolic activation:

2-Aminoanthracene at 10 mcg for all strains

In addition, 2 micromoles crotonaldehyde (dissolved in DMSO) and 1 micromole methyvinyl ketone (in DMSO) are used as special positive controls, in the absence of S-9, to demonstrate the sensitivity of TA-100 in the liquid suspension assay.

Statistical Methods:

Formal statistical methods were not used to evaluate the data. The following requirements generally need to be met for a substance to be characterized as positive:

Doubling of the spontaneous mutation rate.

Dose-response relationship

Reproducibility of the results

Result

:

No cytotoxicity was observed to the bacteria.

The results of the liquid suspension assays conducted on the test material at dose levels ranging from 20 to 5000 microliters per plate in the absence and presence of metabolic activation did not exhibit increased numbers of his⁺ revertant colonies.

The positive control and special positive control treatments in both the nonactivation and S9 activation assays induced large increases in the revertant numbers with the indicator strains, demonstrating the effectiveness of the S9 activation system, the ability of the test system to detect known mutagens, and the sensitivity of this modification for olefinic compounds.

Test substance
Conclusion

:
:

2-Butene-1,4-diol CASNO 110-64-5, Cis 97.5%, Trans 2.0%

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The test material, 2-Butene-1,4-diol, did not exhibit genetic activity in this assay under the test conditions according to the established evaluation criteria.

Reliability : (1) valid without restriction
Guideline study with no deviations.

30.12.2002 (4)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Micronucleus assay
Species : mouse
Sex : male/female
Strain : NMRI
Route of admin. : gavage
Exposure period : once
Doses : 100, 200, 400 mg/kg
Result :
Method : OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year :
GLP : yes
Test substance :

Method : Groups of NMRI mice received single oral-dose administration of 100, 200 or 400 mg/kg test material in distilled water. After a predetermined time, animals were sacrificed, bone marrow was collected, stained and examines according to OECD guideline 474.

Result :
Oral administration of 2-Butene-1,4-diol did not lead to any increase in the number of polychromatic erythrocytes containing either small or large micronuclei. No inhibition of erythropoiesis determined from the ratio of polychromatic to normochromatic erythrocytes was detected.

Test substance : 2-Butene-1,4-diol CASNO 110-64-5 Purity 99.5%
Conclusion :
Under the experimental conditions chosen here, the test substance does not have any chromosome-damaging (clastogenic) effect, and there were no indications of any impairment of chromosome distribution in the course of mitosis.

Reliability : (1) valid without restriction
Guideline study under GLP

Flag : Critical study for SIDS endpoint

30.12.2002 (3)

5.7 CARCINOGENICITY

5. Toxicity

Id 110-64-5

Date 31.12.2002

5.8.1 TOXICITY TO FERTILITY

Type	:	Two generation study
Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	oral unspecified
Exposure period	:	
Frequency of treatm.	:	
Premating exposure period	:	
Male	:	
Female	:	
Duration of test	:	
No. of generation studies	:	
Doses	:	20, 55 or 150 mg/kg-day
Control group	:	
NOAEL parental	:	= 55 mg/kg bw
NOAEL F1 offspring	:	= 55 mg/kg bw
NOAEL F2 offspring	:	= 55 mg/kg bw
Method	:	In a 2-generation oral study, groups of male and female rats received 0, 20, 55, or 150 mg/kg/day, starting when rats were 5 to 6 weeks old for the F0 generation and 22 days old for the F1 generation. Each generation was dosed for at least 80 days before mating.
Remark	:	This study is on the probable main metabolite of 2-Butene-1,4-diol and is supporting.
Result	:	No adverse effects on fertility were noted at doses up to 55mg/kg/day administered over two generations. At 150mg/kg/day, maleic-anhydride was toxic to parental animals. No adverse effects on litter size and on pup survival were noted at doses up to 150mg/kg/day. 55 mg/kg/day appears to be a NOEL.
Test substance	:	Maleic Anhydride CASNO 108-31-6
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint
30.12.2002		(31)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	
Frequency of treatm.	:	
Duration of test	:	
Doses	:	30, 90 pr 140 mg/kg-day
Control group	:	
Method	:	The potential teratogenic and reproductive effects of maleic-anhydride (108316) were investigated. Adult CD-rats approximately 12 weeks of age were used for the teratology study. Female rats were treated orally with 30, 90 or 140mg/kg/day of maleic-anhydride from day six through day 15 of gestation. Females were sacrificed on day 20 of gestation. Fetuses were

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Remark	:	delivered by cesarean section, examined for external abnormalities, soft tissue abnormalities and skeletal abnormalities
Result	:	This study is on the probable main metabolite of 2-Butene-1,4-diol and is supporting.
Test substance	:	An examination of the fetuses did not reveal any effects that were attributed to maleic-anhydride. No increases in fetal malformations were noted, and the variations detected were similar in control and treated groups. Maleic-anhydride was not found to be teratogenic.
Reliability	:	Maleic Anhydride CASNO 108-31-6
Flag	:	(2) valid with restrictions
30.12.2002	:	Acceptable publication
	:	Critical study for SIDS endpoint

(30)

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